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Title: A New On-the-Fly Sampling Method for Incoherent Inelastic Thermal Neutron Scattering Data in MCNP6

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A New On-the-Fly Sampling Method for Incoherent Inelastic Thermal Neutron Scattering Data in MCNP6

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Outline of Topics

- Background: Neutron Scattering at Thermal Energies
- New On-the-Fly Sampling Method
- Preliminary Results for Graphite
  - <u>Eigenvalue</u>: Fuel Compact Benchmarks
  - <u>Surface Current</u>: “Broomstick” Benchmark
- Conclusions
- Next Steps

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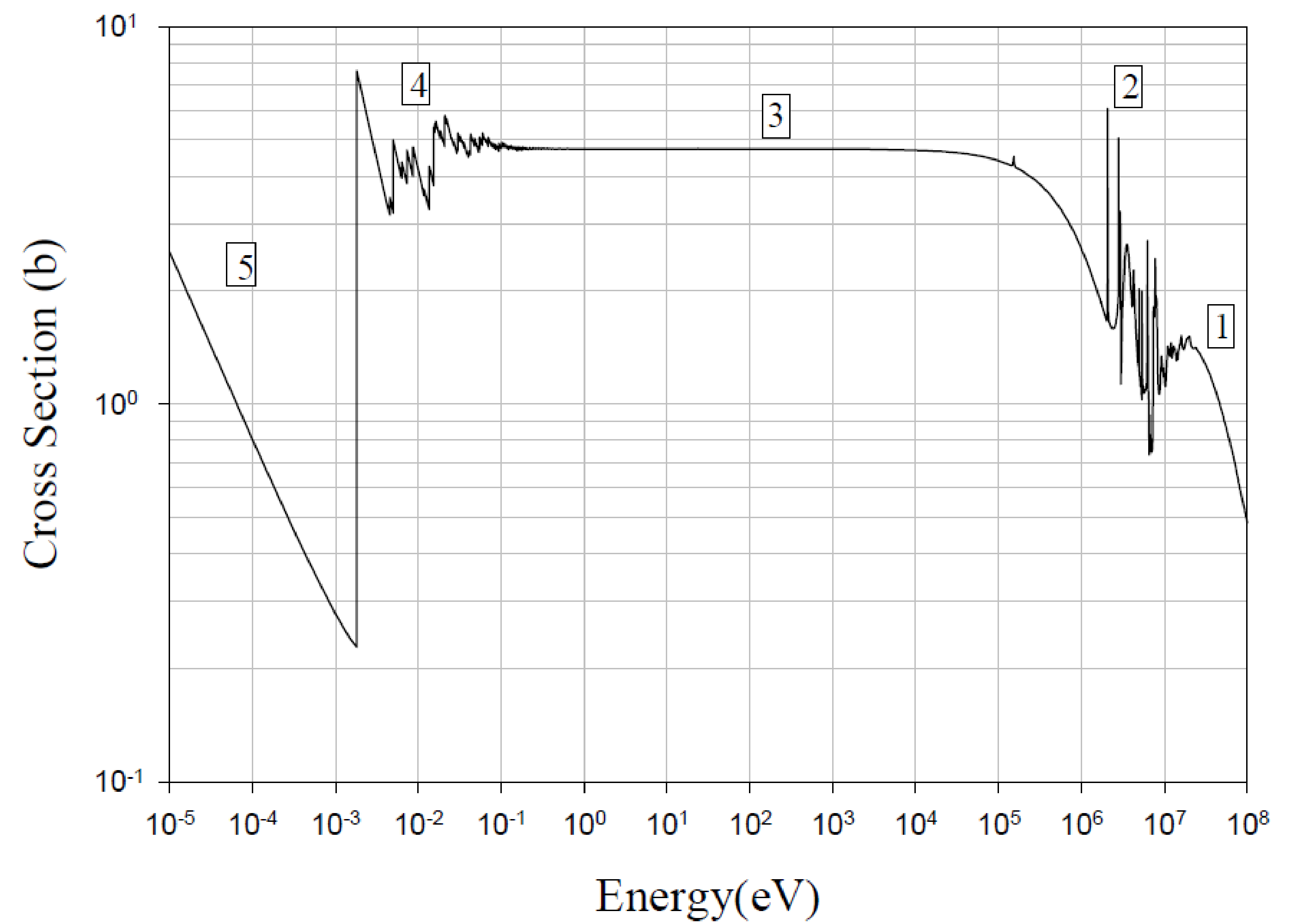
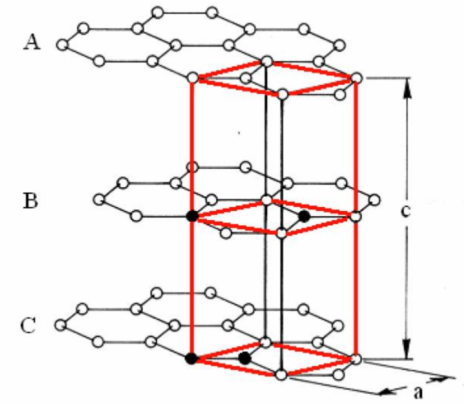
Thermal Neutron Scattering in Graphite

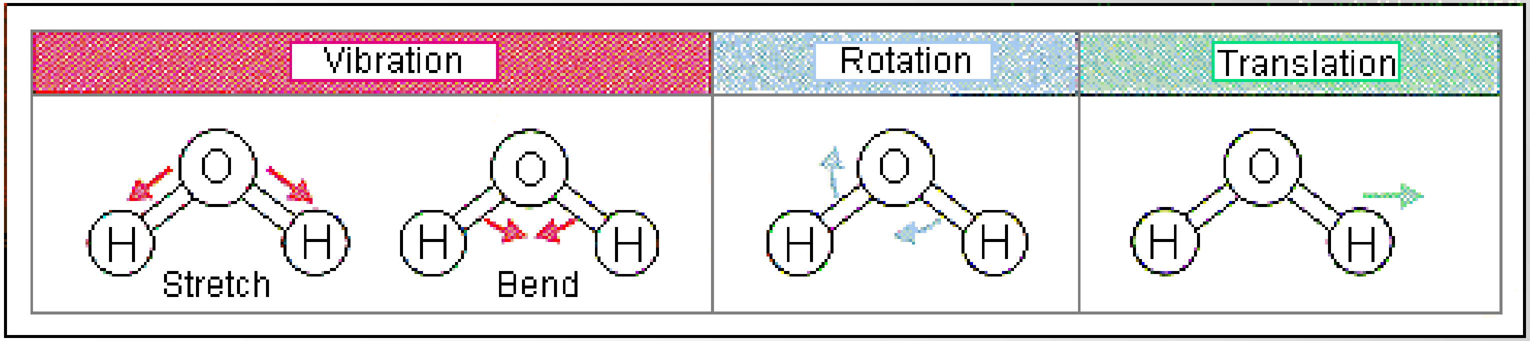


Thermal Neutron Scattering with Materials

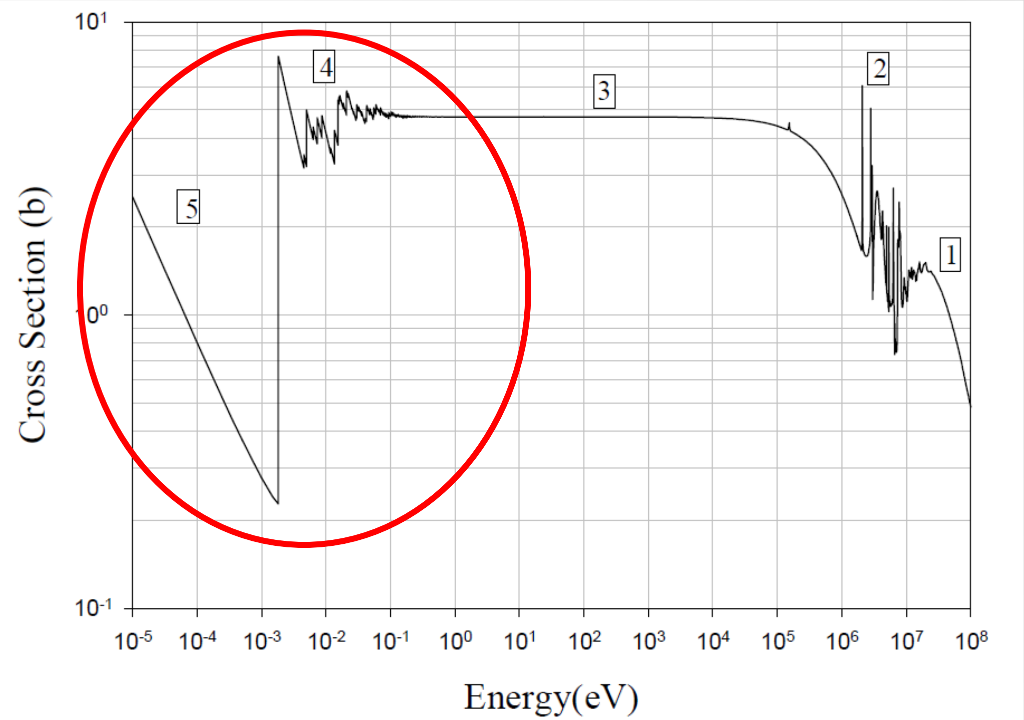
- Thermal neutrons interacting with bound isotopes
- Vibrational, rotational and translational modes (correlated with temperature) affect the scattered neutron energy and angle of scatter after collision



The three Dimensional crystal structure of the graphite hexagonal lattice. The graphite unit cell is shown in red, and its atoms are shown in black solid circles.



Thermal Neutron Scattering in Graphite



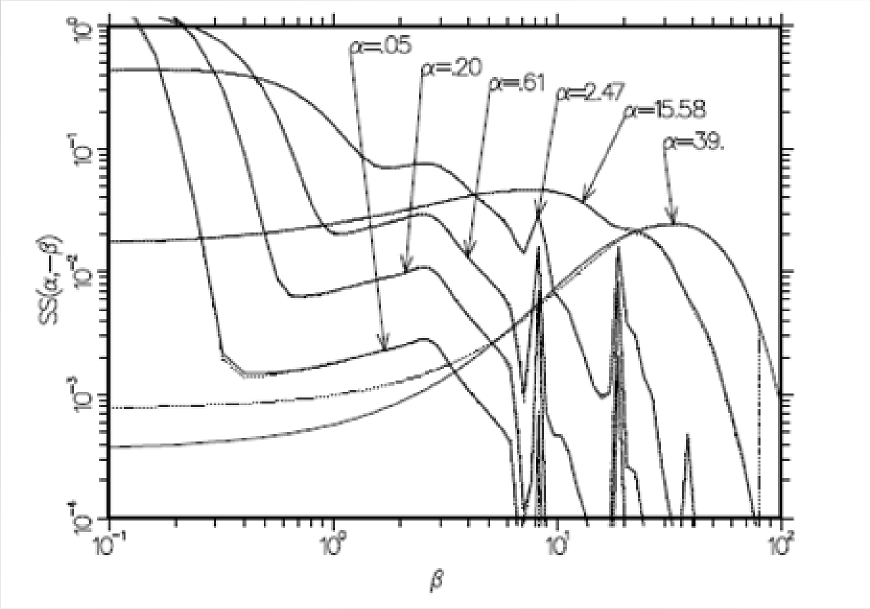
- Region 4: Neutron wavelengths are comparable to interatomic spacing
  - Interactions now take place with a collection of atoms
  - Coherent elastic scattering dominates
- Region 5: Neutron wavelength is larger than the interatomic spacing
  - Incoherent inelastic scattering

Our focus is on incoherent inelastic scattering
Incoherent: ignore interference effects between neutron and target where scattering from different planes of atoms can interfere as neutron wavelength hits different atomic spacings
Inelastic: neutron scatters through a range of energies and angles

Thermal Neutron Scattering with Materials

- The double differential cross section:

$$\sigma(E \rightarrow E', \mu, T) = \frac{\sigma_b}{2kT}\sqrt{\frac{E'}{E}}e^{-\beta/2}S(\alpha,\beta,T)$$



where:

E, E': pre- and post-collision energy
μ: cosine of the scattering angle
σ_b: bound atom scattering cross section
k: Boltzmann constant
T: temperature
S(α,β,T): symmetric form of the scattering law

Thermal Neutron Scattering Data Storage

$$\sigma(E \to E', \mu, T) = \frac{\sigma_b}{2kT}\sqrt{\frac{E'}{E}}e^{-\beta/2}S(\alpha,\beta,T)$$

- α and β are dimensionless quantities representing:

α: momentum transfer

$$\alpha = \frac{E + E' - 2\mu\sqrt{EE'}}{A_0 kT}$$

β: energy transfer

$$\beta = \frac{E' - E}{kT}$$

- S(α,β) ACE datasets from NJOY are large, even for a ***single temperature***:

Material	File Size [MB]
Graphite	24
Water	24.9
U in UO_2	50
O_2 in UO_2	75
Zr in ZrH	56
H in ZrH	116

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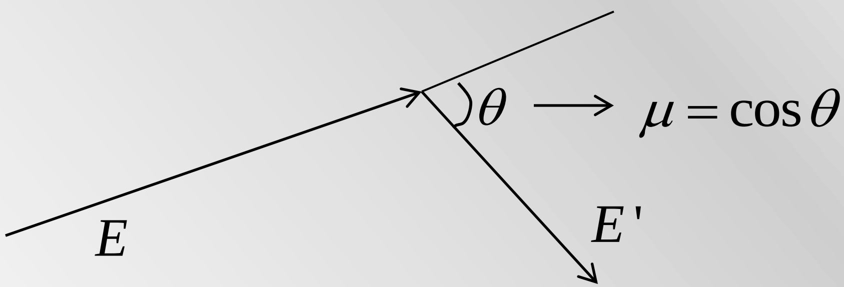
New OTF Strategy at Thermal Energies

- General Monte Carlo sampling procedure for a scattering event



- *E'* and *μ* are random variables and are described by probability density functions (PDFs)

$$f\left(E' \mid E, T\right) \qquad g\left(\mu \mid E \rightarrow E', T\right)$$

- Cumulative distribution functions (CDFs) are provided in the MC code

$$F\left(E' \mid E, T\right) \qquad G\left(\mu \mid E \rightarrow E', T\right)$$

New OTF Strategy at Thermal Energies

- Sample ξ between 0 and 1 and let

$$\xi = F\left(E' | E, T\right)$$

Then

$$E' = F^{-1}\left(\xi | E, T\right)$$

- The sampled *E'* is a function of *T* given the known incoming energy *E* and the sampled ξ. That is, $E'(T|E,\xi)$.
- If we can obtain such a functional expression at different incoming energies and CDF values, we can easily on-the-fly sample the outgoing energy

New OTF Strategy at Thermal Energies

- The Monte Carlo sampling procedure is quite simple:

Sample ξ between [0,1] and then calculate E' based on the expression E'(T|E,ξ) at any temperature.

- Same procedure can be applied to on-the-fly sample μ at any temperature.

$$E'(T|E,\xi)\ ?$$

$$\mu(T|E \rightarrow E',\xi)\ ?$$

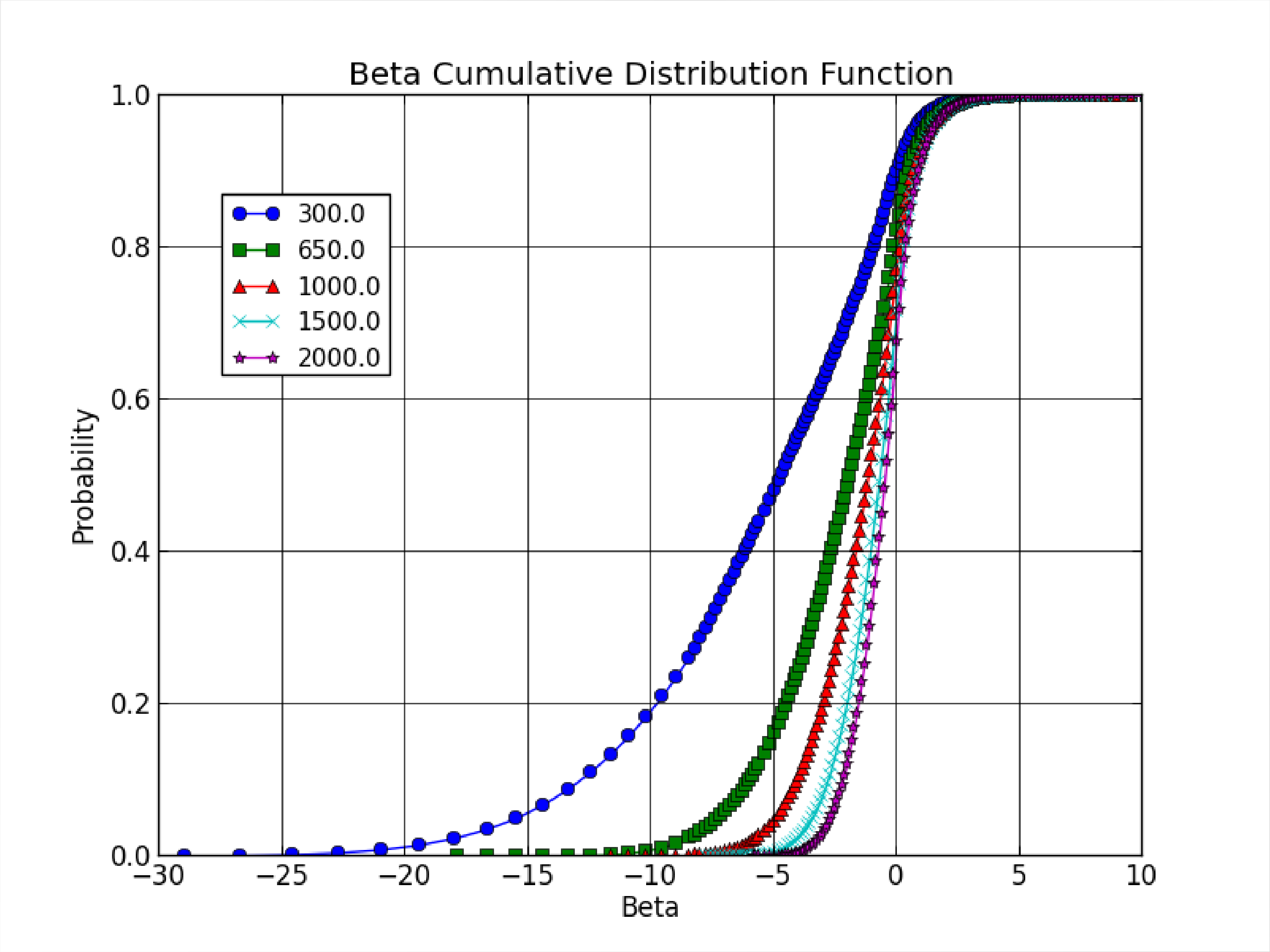
Our Approach

- Current Monte Carlo codes store CDF values in α and β based on S(α,β,T) data at a **single temperature**
  1) α and β are sampled from the CDF at the designated temperature
  2) Linear interpolation in α and β CDFs is used between tabulated values
  3) Scattered energy and angle are calculated from the definitions of α and β

- **Our approach**: **Examine the temperature dependence of α and β CDFs at selected discrete CDF values**
  - Regression analysis performed to find the best temperature fit for a range of temperatures and thermal energies
  - Coefficients of the fits are stored instead of S(α,β,T) data; used to sample scattered energy and angle

β CDF Example

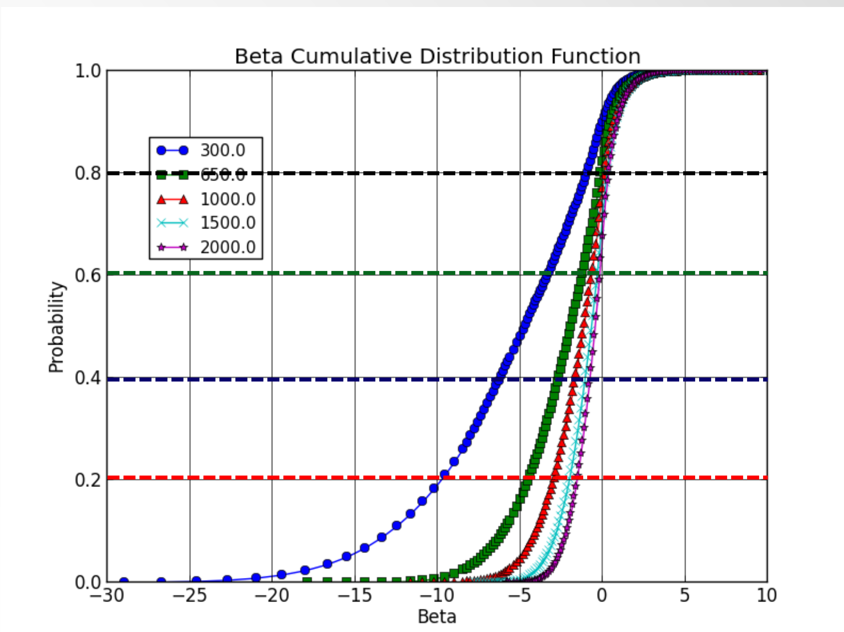
(simplified)

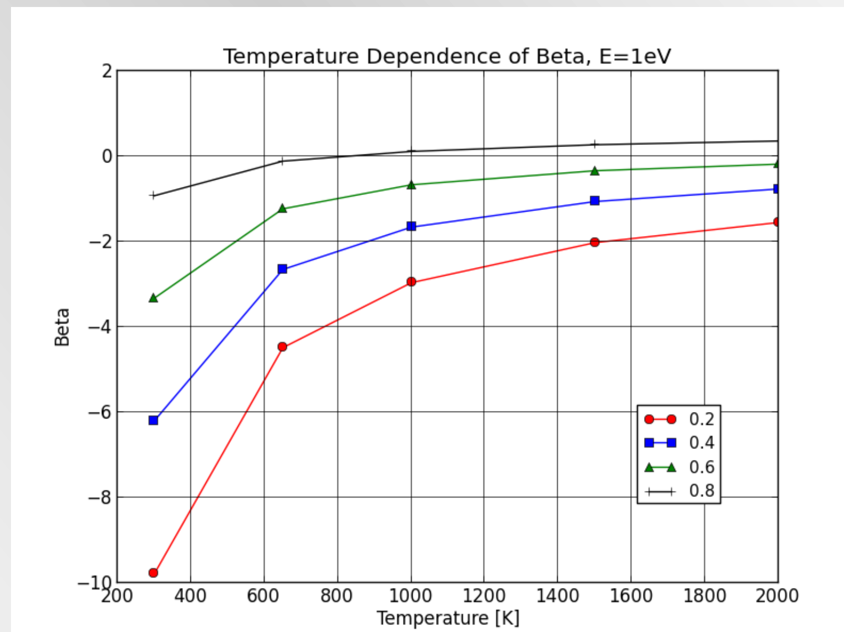


β CDF Example
(simplified)

- Example for Graphite at E = 1 eV for
  - T mesh [300, 650, 1000, 1500, 2000]K
  - β CDF probability line mesh [0.2, 0.4, 0.6, 0.8]

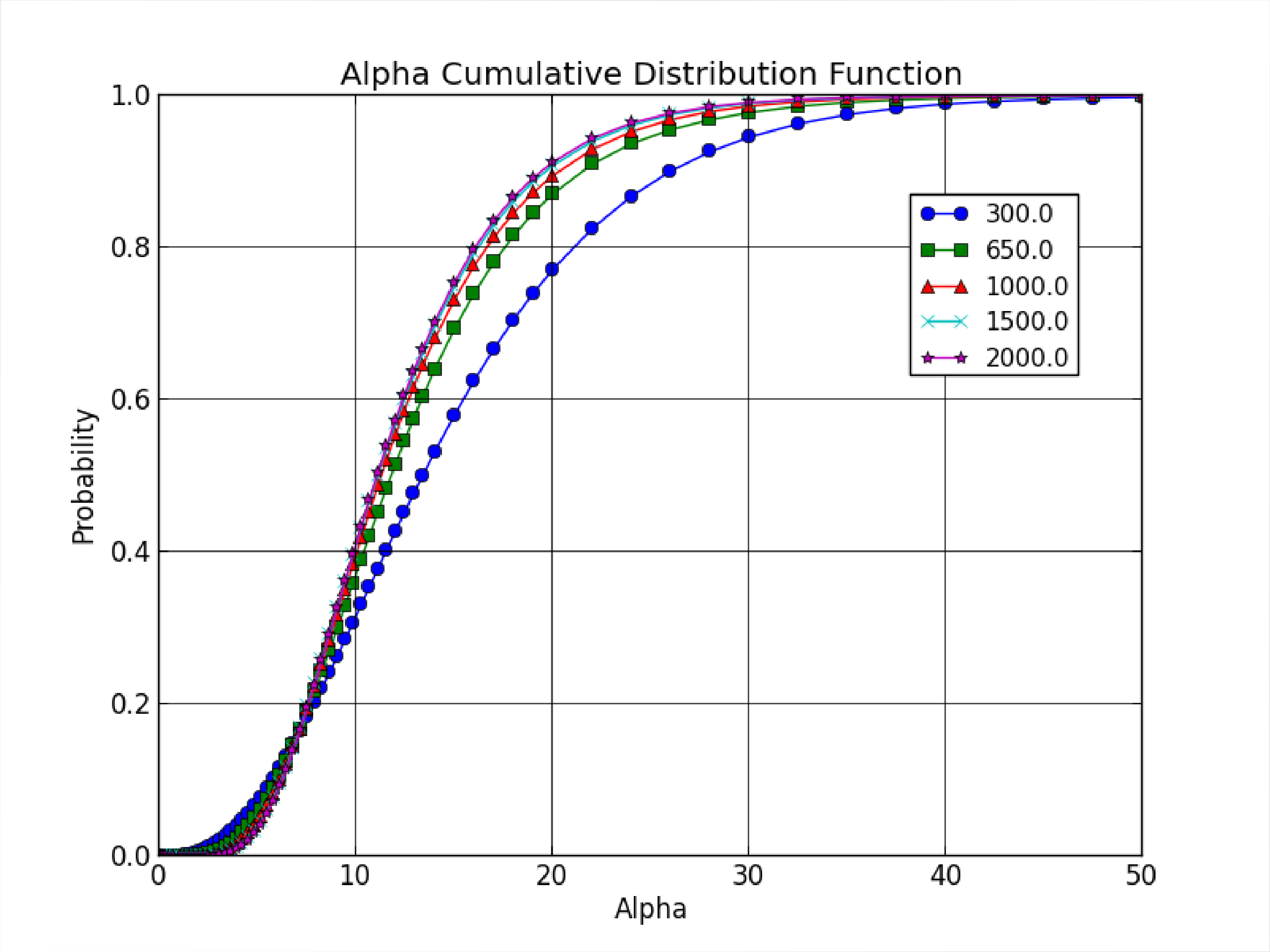
$$\beta(T) \approx \sum_{n=0}^{2} a_n \left(\sqrt{T}\right)^{-n}$$





α CDF Example

(simplified)

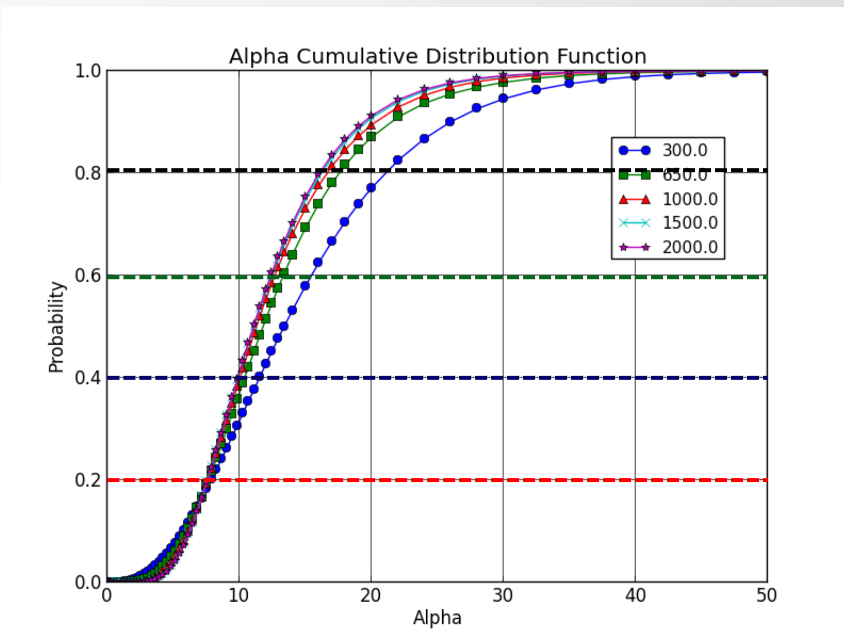


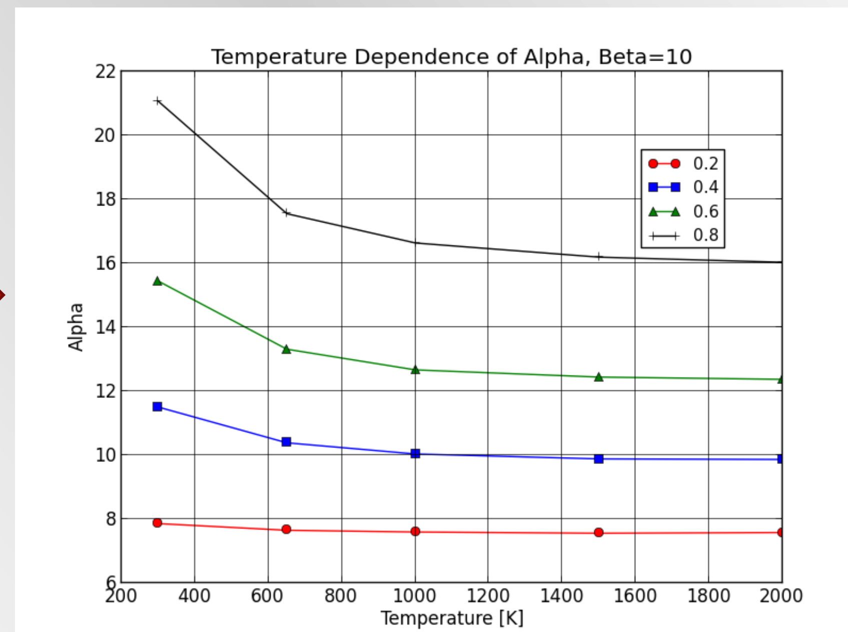
α CDF Example

(simplified)

- Example for Graphite at β = 10 for
  - *T* mesh [300, 650, 1000, 1500, 2000]K
  - α CDF probability line mesh [0.2, 0.4, 0.6, 0.8]

$$\alpha(T) \approx \sum_{n=0}^{4} a_n T^{-n}$$





Total Data Storage

- For Graphite:
  - β coefficients: 190 kB
  - α coefficients: 271 kB

461 kB

- Assuming cross section data needed at ~100 temperatures for a problem:
  - Graphite: data storage reduction of around ***5,331x***

Sampling β from Coefficient File

ENERGY$_i$	**$a_{n,1}$**	**$a_{n,2}$**	**$a_{n,3}$**
P_1	a_{11}	a_{12}	a_{13}
P_2	a_{21}	a_{22}	a_{23}
P_3	a_{31}	a_{32}	a_{33}
…	…	…	…
P_N	a_{n1}	a_{n2}	a_{n3}

ENERGY$_{i+1}$	**$a_{n,1}$**	**$a_{n,2}$**	**$a_{n,3}$**
P_1	a_{11}	a_{12}	a_{13}
P_2	a_{21}	a_{22}	a_{23}
P_3	a_{31}	a_{32}	a_{33}
…	…	…	…
P_N	a_{n1}	a_{n2}	a_{n3}

. . .

ENERGY$_N$	**$a_{n,1}$**	**$a_{n,2}$**	**$a_{n,3}$**
P_1	a_{11}	a_{12}	a_{13}
P_2	a_{21}	a_{22}	a_{23}
P_3	a_{31}	a_{32}	a_{33}
…	…	…	…
P_N	a_{n1}	a_{n2}	a_{n3}

Sampling Procedure:

1) Use incident energy to determine appropriate section of file

$$E_i < E < E_{i+1}$$

2) Sample probability line

$$P_i < \xi < P_{i+1}$$

3) Use temperature to calculate β at:

$$(E_i, P_i), (E_i, P_{i+1}), (E_{i+1}, P_i), (E_{i+1}, P_{i+1})$$

4) Linearly interpolate between four sets to obtain sampled β

Sampling α from Coefficient File

β_i	$a_{n,1}$	$a_{n,2}$	$a_{n,3}$
P_1	a_{11}	a_{12}	a_{13}
P_2	a_{21}	a_{22}	a_{23}
P_3	a_{31}	a_{32}	a_{33}
…	…	…	…
P_N	a_{n1}	a_{n2}	a_{n3}

B_{i+1}	$a_{n,1}$	$a_{n,2}$	$a_{n,3}$
P_1	a_{11}	a_{12}	a_{13}
P_2	a_{21}	a_{22}	a_{23}
P_3	a_{31}	a_{32}	a_{33}
…	…	…	…
P_N	a_{n1}	a_{n2}	a_{n3}

. . .

β_N	$a_{n,1}$	$a_{n,2}$	$a_{n,3}$
P_1	a_{11}	a_{12}	a_{13}
P_2	a_{21}	a_{22}	a_{23}
P_3	a_{31}	a_{32}	a_{33}
…	…	…	…
P_N	a_{n1}	a_{n2}	a_{n3}

Sampling Procedure:

1) Use sampled beta to determine appropriate section of file

$$\beta_i < \beta < \beta_{i+1}$$

2) Sample probability line

$$P_i < \xi < P_{i+1}$$

3) **Calculate α bounds based on incident energy and sampled β. Then, adjust ξ to the bounds**

4) Use temperature to calculate α at:

$$(\beta_i, P_i), (\beta_i, P_{i+1}), (\beta_{i+1}, P_i), (\beta_{i+1}, P_{i+1})$$

5) Linearly interpolate between four sets to obtain sampled β

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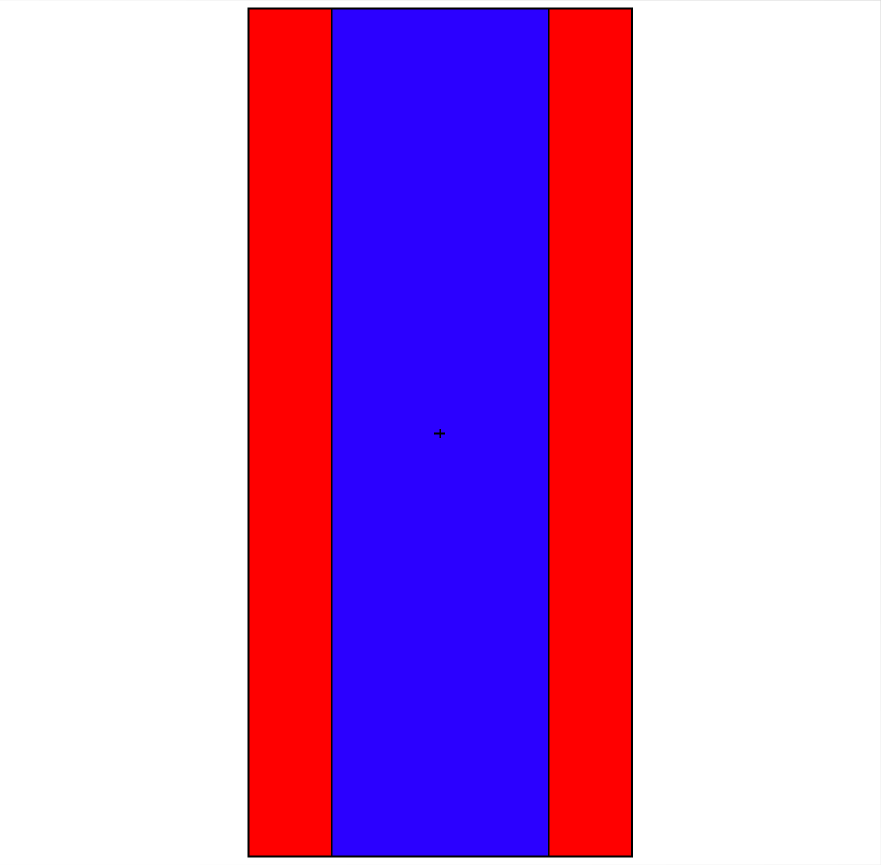
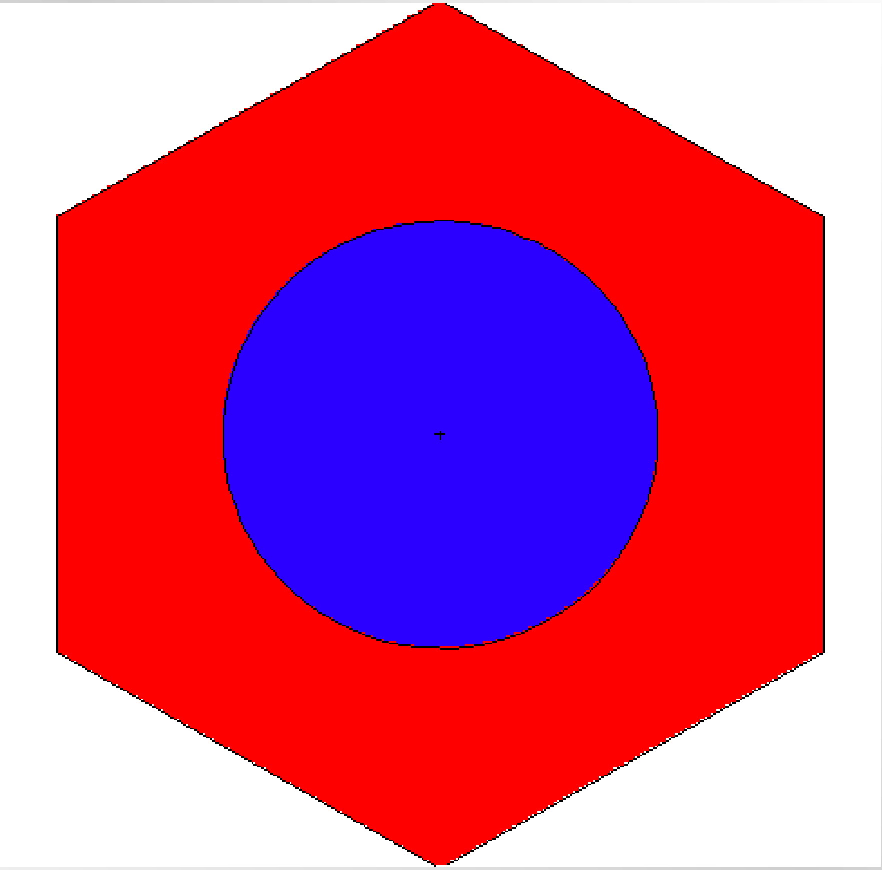
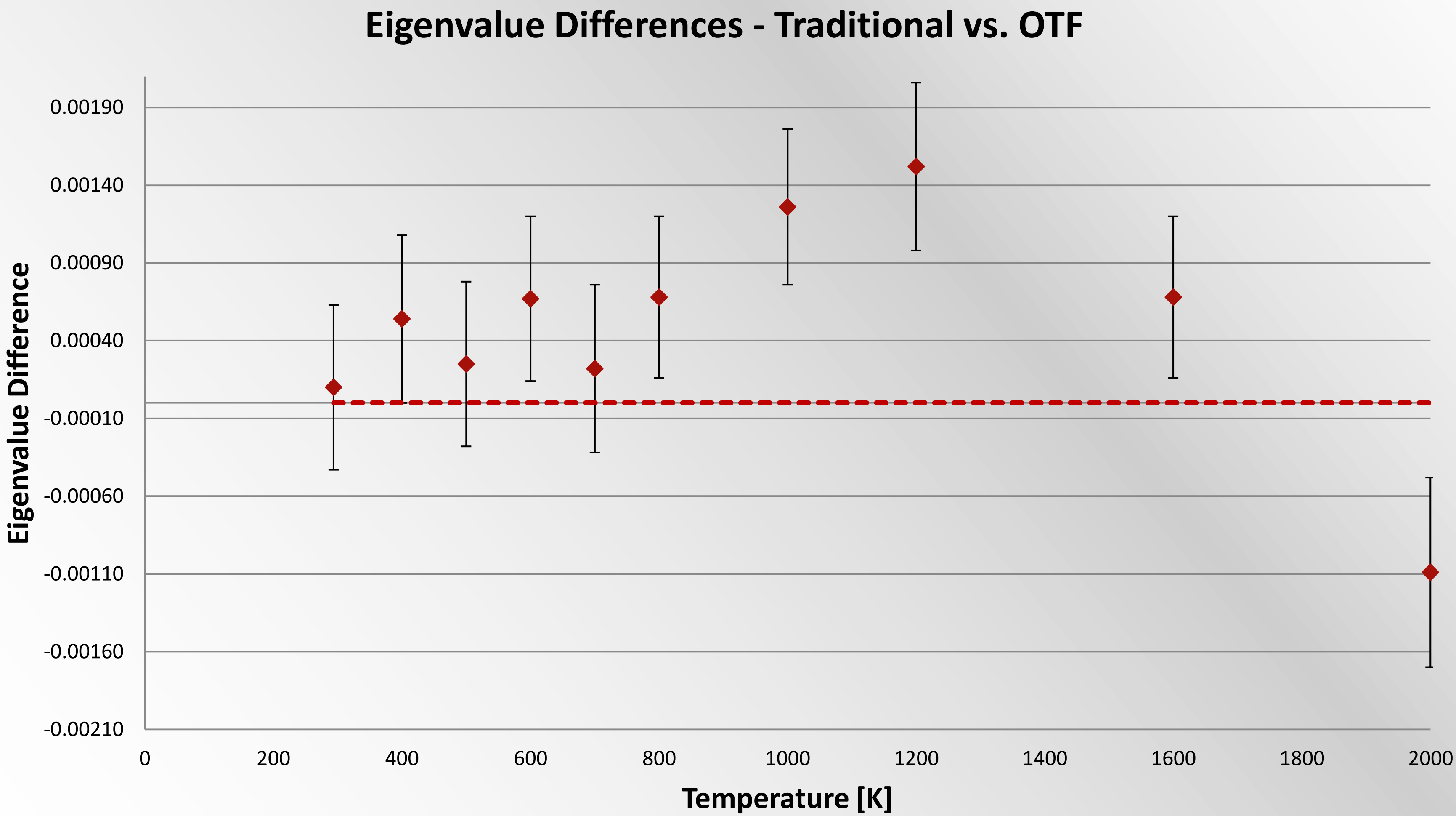
NGNP Homogeneous Fuel Compact





Eigenvalue Results

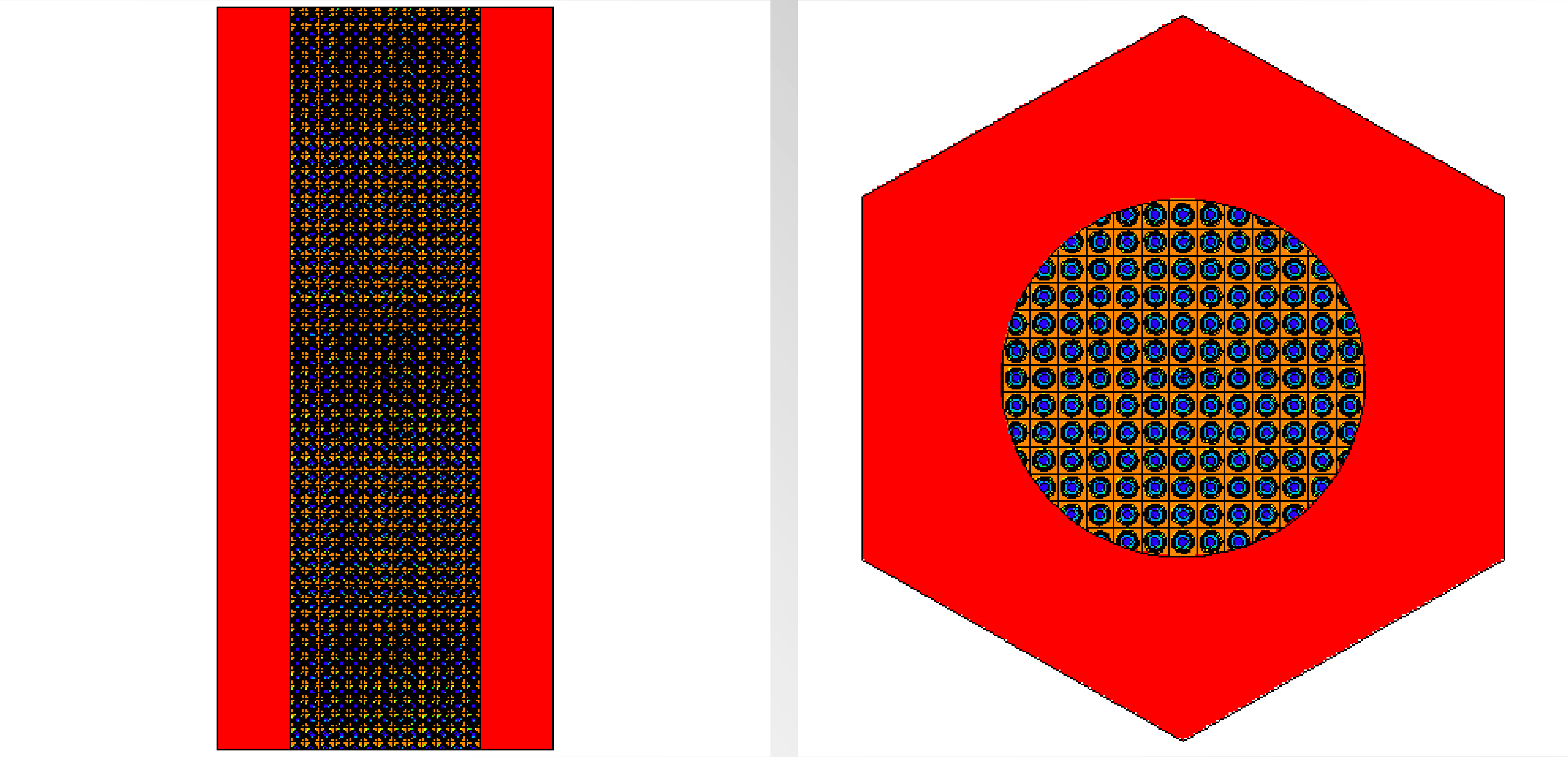


Eigenvalue Results

	Traditional S(α,β)	OTF S(α,β)	Relative Difference
293.6 K	1.28625(37)	1.28615(38)	0.00010(53)
400 K	1.28397(40)	1.28343(37)	0.00054(54)
500 K	1.28165(37)	1.28140(38)	0.00025(53)
600 K	1.27950(37)	1.27883(38)	0.00067(53)
700 K	1.27658(37)	1.27636(39)	0.00022(54)
800 K	1.27449(36)	1.27381(37)	0.00068(52)
1000 K	1.27147(35)	1.27021(36)	0.00126(50)
1200 K	1.26768(38)	1.26616(38)	0.00152(54)
1600 K	1.26164(39)	1.26096(35)	0.00068(52)
2000 K	1.25570(37)	1.25679(37)	-0.00109(52)

No S(α,β) Treatment: $k = 1.29119(37)$

NGNP Heterogeneous Fuel Compact



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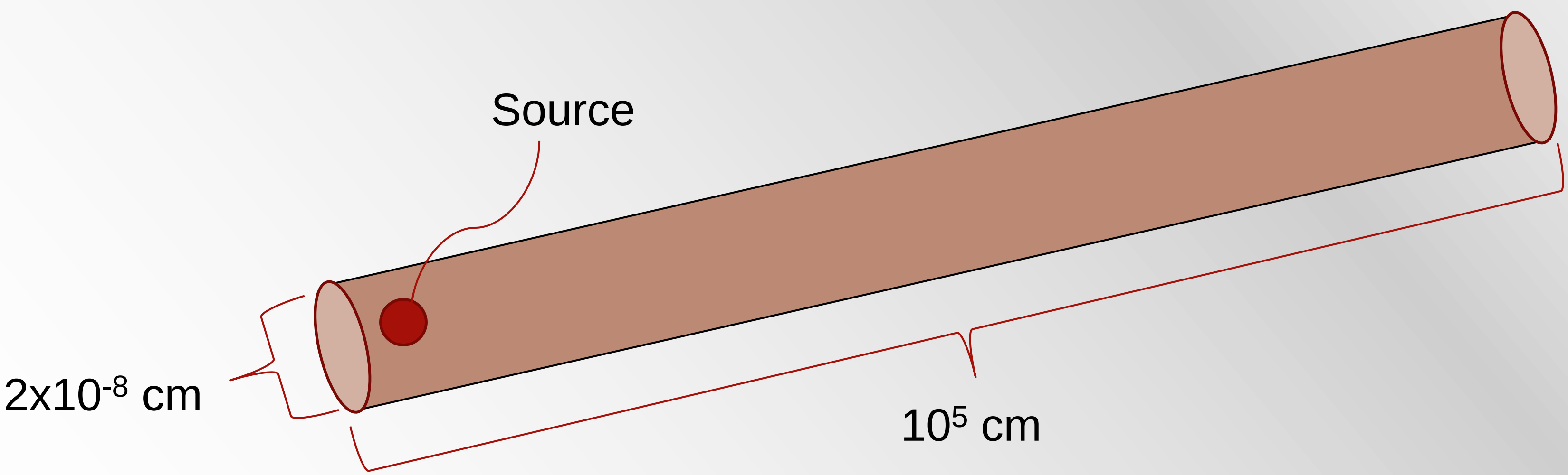
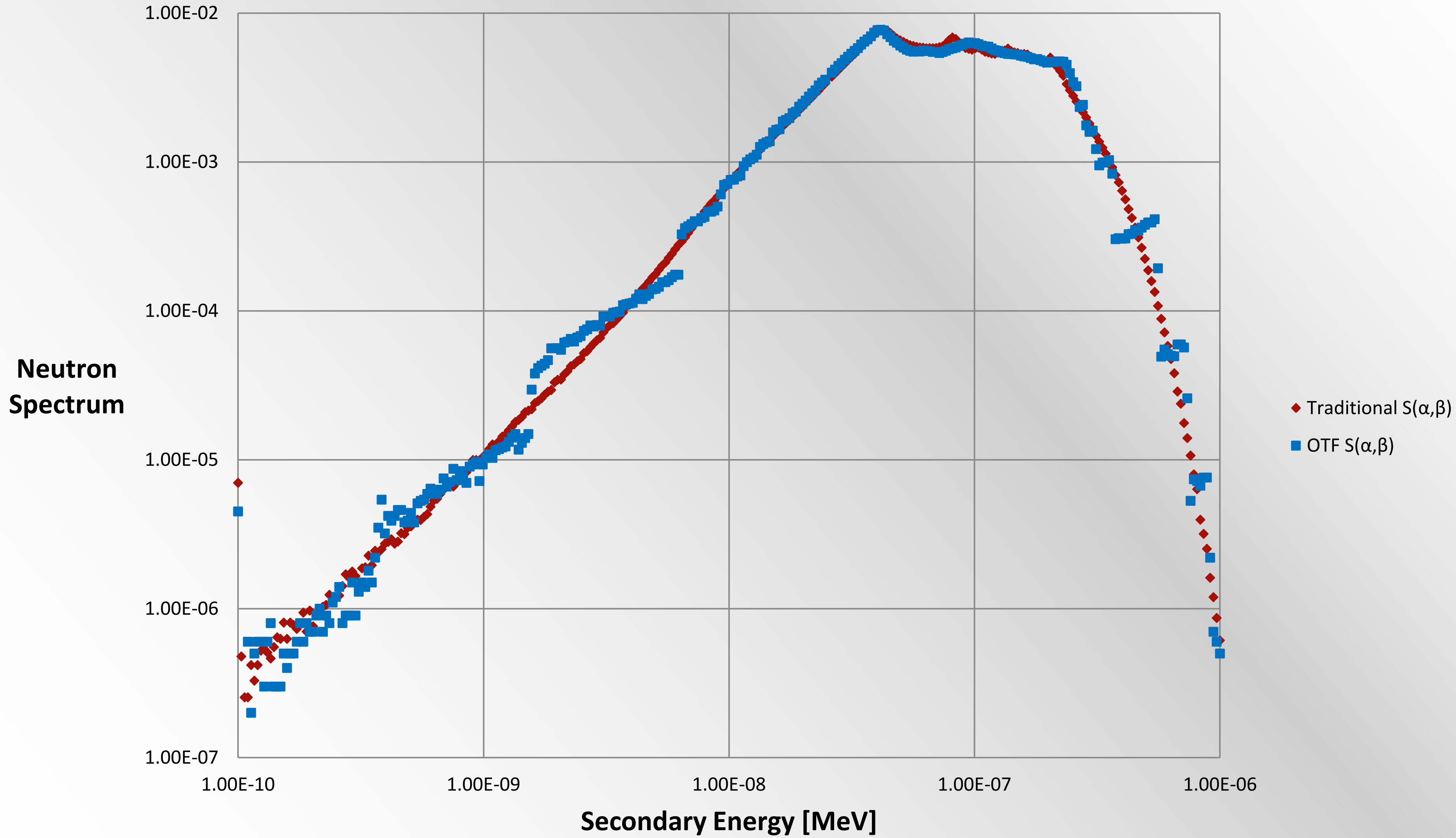
Broomstick Benchmark Problem

- Very thin, very long cylinder with monoenergetic source along axis
- Vacuum outside cylinder
- Tallies taken on planes perpendicular to cylinder
- Capable of detecting single scatterers – very sensitive to S(α,β)



Broomstick Problem: Secondary Neutron Spectrum

Graphite: 2000K, E = 0.0253 eV



Outline of Topics

- Introduction and Background
- Construction of Energy and Momentum Transfer PDFs/CDFs
- Temperature Dependence of the CDFs
- Functional Fittings of the Temperature-Dependent CDFs
- **Conclusions and Future Work**

Summary

- On-the-fly sampling methods have been developed to reduce cross section storage for Monte Carlo codes
- Temperature dependence of S(α,β,T) data ***cannot*** be fit with functions
- Our work examines the temperature dependence of CDFs in energy transfer (β) and momentum transfer (α)
- The neutron's outgoing energy and flight angle after a thermal scattering event at an arbitrary temperature are sampled on-the-fly
  - Eliminates the need to store S(α,β,T) data at discrete temperatures
- Preliminary benchmark tests show good agreement at specific temperatures and energies – **many improvements still need to be made**
- Total storage of coefficients is ***461 kB*** for graphite (includes all temps)
  - Current storage method is ***24 MB per temperature***

Future Work

- Optimize the energy, temperature and CDF probability meshes
  - Choose values such that linear interpolation between values gives good results within some fractional tolerance
  - May need finer meshes in certain regions and coarser meshes elsewhere – dependent on phonon frequency distribution
- Examine more basis functions for the regression analysis
  - Is there a link between the basis function and the underlying physics in the thermal energy range?
- Extend analysis to other moderator materials
- Test the coefficients in a ***realistic*** reactor problem to see how eigenvalue, flux, coefficients of reactivity, etc. are affected by small differences in scattered energy and flight angle

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